

ACCESSIBILITY CORRECTION FACTORS FOR ELECTRONIC MODELS OF CYTOCHROME P450 METABOLISM

ABSTRACT OF THE DISCLOSURE

Accessibility correction factors may be used to modify values predicted by models of electronic component substrate reactivity. Most of the correction factors described herein pertain to either steric or orientation effects on substrate accessibility. The correction factors may be derived from one or more "descriptors" of the substrate structure. Each group of descriptors and associated correction factor pertain to a particular site on the substrate. Examples of such descriptors include site polarity, protrusion, partial surface area, partial charge, etc. Often the correction factor is a function of multiple descriptors. The function may be an expression comprising multiple terms, each representing the weighted contribution of a particular descriptor. In other embodiments, the correction factor is simply a descriptor or a descriptor multiplied by a coefficient or other function.